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Soutiendra sa thèse le mercredi 30 octobre 2013 à 13h00

Amphi Monge - École Polytechnique- Palaiseau

Damping, satellites and multiple excitations in oxides and nanostructures: efficient theoretical and numerical approaches towards a dynamical many-body theory

Finding alternative sources of energy is one of the challenges of the XXIst century. Solar energy, thanks to photovoltaic phenomenon, appears to be very promising.
In solar cells, the absorbed photon creates an electron-hole pair. These two charge carriers, once separated, can be collected to produce current. A way to increase the efficiency of this process is to take benefit of the multiple exciton generation. For instance, in the impact ionisation mechanism, a high energy photon excites an electron to a high energy state (hot electron) which can de-excite by the conversion of part of its energy into the production of other electron-hole pairs. Due to the confinement, this effect is expected to be enhanced in nano-objects where the electronic properties, like for example the absorbed energy, can be tuned by playing with controllable parameters as, e.g. the size.
Multiple excitation is only one example of phenomena which can be described in theoretical ab initio spectroscopy only by including dynamical effects in the calculation of absorption. These dynamical effects lead also to the renormalization of the absorption peaks (damping) or the occurrence of plasmon satellites in photoemission spectra. The aim of this thesis has been to devise a dynamical theory of absorption in the context of many-body perturbation theory and to study the impact of dynamical effects on the spectral properties of nanostructured objects.
The latter aspect has been studied on carbon-based structures. Since dynamical effects are carried out by the frequency dependence of the inverse dielectric matrix ε^{-1}, we discussed electron energy loss spectra (EELS), corresponding to the diagonal part of ε^{-1}, and the spectral function (related to the self-energy).
Different stacking of bulk graphite have been investigated as well as the evolution of the spectrum from bulk graphite to the isolated graphene sheet. The latter analysis is usually carried out with the supercell method and therefore it can not naively be pushed to far, since all the parameters of the calculation grow with the volume of the cell. Thus a Coulomb cutoff method has been implemented in the simulation codes DP and EXC, in order to achieve the calculation of the properties of the isolated system with a small computational effort. This implementation allowed the calculation of the EEL spectra and the spectral function of the truly isolated graphene for an interlayer distance of only twice the bulk's one and with a reduced k-point mesh.
On the other hand, state of the art calculations of the dielectric response and of the absorption spectrum rely on the Bethe-Salpeter equation (BSE), which describes the explicit electron-hole interaction. The latter is expressed by the statically screened Coulomb interaction W, which enters in the two-particle correlation function L.
Starting from the equation of motion of the Heisenberg creation and annihilation field operators, and using the Schwinger equation to define the two-particle correlation function L, I obtained a differential equation for L which has exactly the same physical content as the full BSE, but has the advantage that the dynamical contributions of W do not need to be approximated. The solution includes dynamical effects of W to all orders, and the derivation treats on the same footing the contributions from the single-particle excitations and from the e-h interaction.

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